

Acetaldehyde

75-07-0 | DTXSID5039224

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 13.1 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.79e-01

Confidence level: 6.96e-01

Nearest Neighbors from the Training Set

Image not found

Acetaldehyde

Measured: 22.7

Predicted: 13.1

Image not found

Acrolein

Measured: 3.78

Predicted: 5.11

Image not found

Propanal

Measured: 5.27

Predicted: 3.91

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Acetone

Measured: 17.2

Predicted: 6.59

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Formaldehyde

Measured: 13.2

Predicted: 11.9